

The effects of next to nearest neighbor hopping on Bose-Einstein condensation in cubic lattices

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Abstract. In this paper, we present results of our calculations on the effects of next to nearest neighbor boson hopping (t') energy on Bose-Einstein condensation in cubic lattices. We consider both non-interacting and repulsively interacting bosons moving in the lowest Bloch band. The interacting bosons are studied making use of the Bogoliubov method. We find that the bose condensation temperature is enhanced with increasing t' for bosons in a simple cubic (sc) lattice and decreases for bosons in body-centered cubic (bcc) and face-centered cubic (fcc) lattices. We also find that interaction induced depletion of the condensate is reduced for bosons in a sc lattice while is enhanced for bosons in bcc and fcc lattices.

Keywords. Bose-Einstein condensation, Optical lattice

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1. Introduction

Studies of Bose-Einstein condensation in optical lattices and crystalline lattices is an active field of research both in atomic [1–4] and condensed matter physics [5–11]. In condensed matter physics, there have been extensive studies of bose condensation of bipolarons [5], excitons [6], exciton-polaritons [7,8], and magnons [9–11]. Studies of bosons in optical lattices may be said to have received a boost with the demonstration of bose condensed to Mott insulator transition [2] predicted in theoretical studies [1,12–15] of strongly interacting lattice bosons. In the presently available optical lattices, it has been shown [1] that it is sufficient to include nearest-neighbor (NN) hopping of bosons in the kinetic energy part of the Hamiltonian of the system. Nevertheless, considering the fast pace of developments in this field, it may be useful to investigate the effects of the next to nearest-neighbor (NNN) hopping on bose condensation in optical and crystalline lattices. Recently, we presented a study of the lattice symmetry effects on bose condensation in cubic lattices [16]. In that work, we had confined to NN hopping of lattice bosons. In this paper, we extend this work including NNN boson hopping. The bosons are considered to be of spin-zero and charged (see also the note in Ref. [17]). We would like to emphasize that we are not exclusively considering bosons in optical lattices. Our calculations should be considered in the enlarged context including bose condensation in crystalline lattices. In the next section, we describe the models and methods used in our calculations along with a discussion of results. The conclusions are given Sec. III.

2. Bose condensation in cubic lattices with NNN hopping

Non-interacting bosons: Consider bosons moving in cubic lattices. The energy eigenfunctions of a single boson moving in a periodic optical or crystalline lattice potential are Bloch waves [18] and energy eigenvalues form bands. The Hamiltonian of non-interacting bosons in an energy band is:

$$H = \sum_k [\epsilon(k) - \mu] c_k^\dagger c_k, \quad (1)$$

where $\epsilon(k)$ is the one-boson energy band structure, k is the boson quasi-momentum, μ is the chemical potential, and c_k^\dagger is a boson creation operator. Within a tight-binding approximation scheme [19], including the NN and the NNN Wannier functions overlaps, the s-band structures we consider for cubic lattices are:

$$\begin{aligned} \epsilon_{sc}(k_x, k_y, k_z) = & -2t \sum_{\mu=x}^z \cos(k_\mu) \\ & - 2t' \sum_{\mu=x}^z \sum_{\mu \neq \nu, \nu=x}^z \cos(k_\mu) \cos(k_\nu), \end{aligned} \quad (2)$$

$$\begin{aligned} \epsilon_{bcc}(k_x, k_y, k_z) = & -8t \prod_{\mu=x}^z \cos\left(\frac{k_\mu}{2}\right) \\ & - 2t' \sum_{\mu=x}^z \cos(k_\mu), \end{aligned} \quad (3)$$

$$\begin{aligned} \epsilon_{fcc}(k_x, k_y, k_z) = & -2t \sum_{\mu=x}^z \sum_{\mu \neq \nu, \nu=x}^z \cos\left(\frac{k_\mu}{2}\right) \cos\left(\frac{k_\nu}{2}\right) \\ & - 2t' \sum_{\mu=x}^z \cos(k_\mu), \end{aligned} \quad (4)$$

where the lattice constant has been set to unity. Here t is NN boson hopping energy and t' is NNN boson hopping energy in the lattice.

The condensation temperature T_B for bosons in these bands can be calculated from the boson number equation

$$n = \frac{1}{N_x N_y N_z} \sum_{k_x} \sum_{k_y} \sum_{k_z} \frac{1}{e^{\frac{\epsilon(k_x, k_y, k_z) - \mu}{k_B T}} - 1}, \quad (5)$$

where $N_s = N_x N_y N_z$ is the total number of lattice sites, k_B is the Boltzmann constant, T is the temperature, and n is number of bosons per site. We have numerically solved the bosons number equation (Eq. 5) to obtain the bose condensation temperature and ground state occupancy. The results of these calculations for various lattices considered are shown

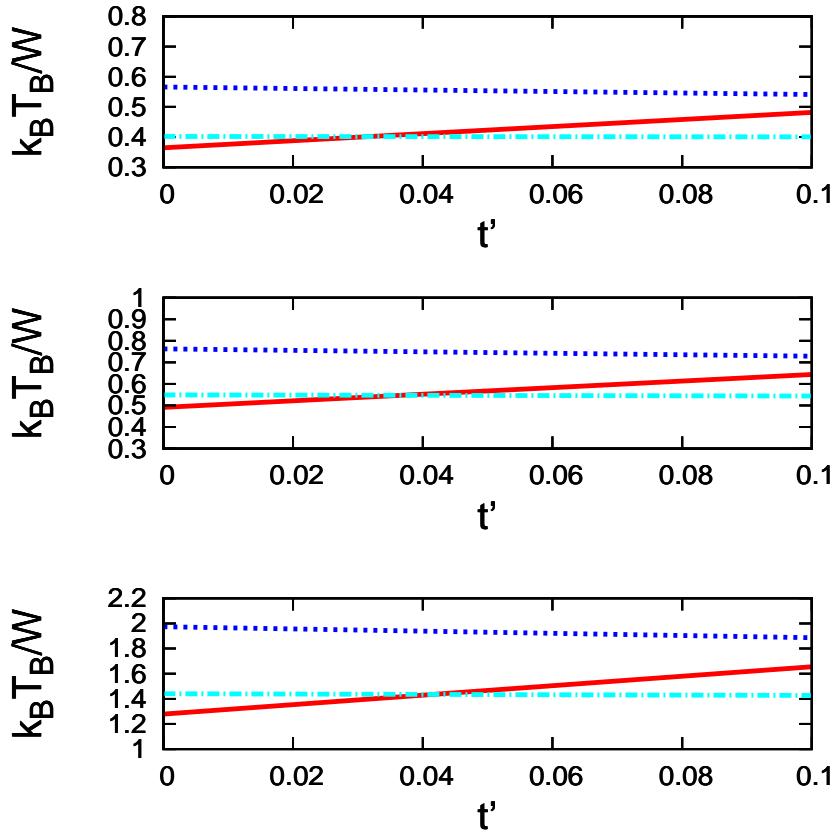


Figure 1. The bose condensation temperature vs NNN hopping t' for noninteracting bosons in various cubic lattices. The curves are shown for: sc (solid line), bcc (dotted line), and fcc (dash-dot line). These results are for $n = 0.25$ (top panel), $n = 0.4$ (middle panel), $n = 1.5$ (bottom panel). In this and other figures W is the half-band-width.

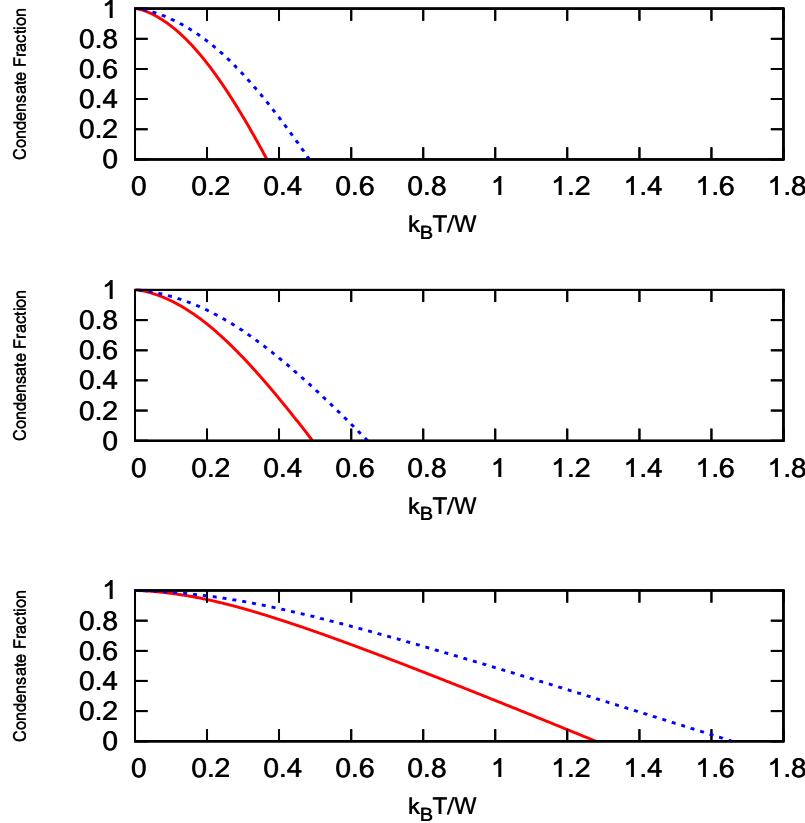


Figure 2. The variation of condensate fraction with temperature (T) for bosons in a sc lattice with NNN hopping $t' : t' = 0$ (solid line), $t' = t/10$ (dotted line). Here $n = 0.25$ (top panel), $n = 0.4$ (middle panel), $n = 1.5$ (bottom panel).

in Fig. 1. We find that t' increases the bose condensation temperature of bosons in a sc lattice. For bosons in bcc lattice the T_B decreases with increasing t' . For bosons in a fcc lattice also increasing t' more or less leave T_B unaltered. These trends can be approximately understood in the low boson density limit. In this limit, states with significant thermal population is close to the bottom of the energy bands. Now, for a given small boson density, the ratio between bose condensation temperature and half-band-width is proportional to $1/(m^*W)$, where m^* is the boson effective mass. We find that, in the low density limit, T_B/W (where T_B is the bose condensation temperature and W is the half-band-width) goes as: $(t + 4t')/3t$ for sc, $(t + t')/(2t + 3t')$ for bcc, and $1/3$ for fcc. On plotting, one can easily see that the T_B/W increases with t' in the sc case, decreases slightly for bcc case, and remains constant for the fcc case. These trends are consistent with our numerical results.

The growth of the condensate fraction and the number dependence of T_B for bosons in

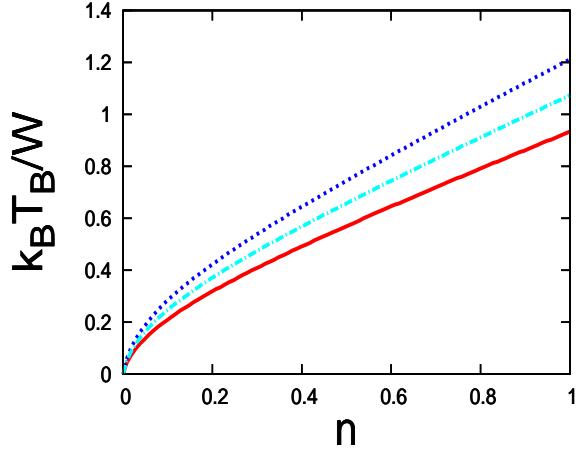


Figure 3. The bose condensation temperature vs n for bosons in a sc lattice with NNN hopping $t' : t' = 0$ (solid line), $t' = t/20$ (dash-dot line), $t' = t/10$ (dotted line).

a sc lattice shown in Fig. 2 and Fig. 3 are similar to that found for the case of $t' = 0$ [16]. Similar results are obtained (not shown) for bosons in bcc and fcc lattices.

Interacting bosons: The Hamiltonian of interacting bosons is

$$H = \sum_k [\epsilon(k) - \mu] c_k^\dagger c_k + \frac{U}{2N_s} \sum_k \sum_{k'} \sum_q c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k, \quad (6)$$

where U is a constant boson-boson repulsive interaction energy. To treat the effect of interactions we make use of Bogoliubov approach [20] to the interacting bosons system. In this theory, it is assumed that the ground state of interacting bosons system is a bose condensate. Since the condensation occurs into the lowest single particle state (for which $\mathbf{k} = 0$ in our cases), one gets $\langle c_0^\dagger c_0 \rangle \approx \langle c_0 c_0^\dagger \rangle$. This allows one to treat the operators c_0^\dagger and c_0 as complex numbers and one gets $\langle c_0^\dagger \rangle = \langle c_0 \rangle = \sqrt{N_0}$. Here $N_0 = n_0 N_s$ in which n_0 is the boson occupancy per lattice site in the $\mathbf{k} = 0$ state. The second order interaction terms are obtained from the substitution: $c_0^\dagger \rightarrow \sqrt{N_0} + c_0^\dagger$. On using this approach, the boson number equation is obtained to be (for details see Ref. 16):

$$\begin{aligned} n = n_0 + \frac{1}{2N_s} \sum'_k & \left[\left(1 + \frac{\xi(k) + Un_0}{E(k)} \right) \times \frac{1}{e^{\frac{E(k)}{k_B T}} - 1} \right] \\ & + \frac{1}{2N_s} \sum'_k \left[\left(1 - \frac{\xi(k) + Un_0}{E(k)} \right) \times \frac{1}{e^{\frac{-E(k)}{k_B T}} - 1} \right], \end{aligned} \quad (7)$$

where $\xi(k) = \epsilon(k) - \epsilon_0$, ϵ_0 is the energy of the lowest single particle state, and $E(k) = \sqrt{\xi^2(k) + 2Un_0\xi(k)}$. The primes on the summation signs indicates that the sums excludes the $\mathbf{k} = 0$ state in to which the bosons condense. The Bogoliubov method used would valid so long as the interaction energy is smaller than the kinetic energy of the bosons.

This approximately translates to $U \leq 2W$. The effect of increasing interaction (U) is to lead to an increase in the effective mass of the bosons which eventually gets localized for large interaction strengths. But, this happens for integer filling. Our results (Figs. 4-6) are for $n = 0.25, 0.4$, and 1.5 which is not close to integer filling. The interaction induced enhancement of the boson effective mass will not be significant in this case since there are sufficient number of un-occupied sites in the lattice so that the bosons can move around without paying a penalty for multiple boson site occupancies. The condensate fraction for bosons in various cubic lattices are shown in Fig. 4-6.

For bosons in a sc lattice, we find that interaction induced depletion of the condensate is reduced with increasing t' as shown in Fig. 4. For bosons in a bcc lattice (Fig. 5), increasing t' is found increase the interaction induced depletion. In the case of bosons in an fcc lattice, the effects of increasing t' does not have much effect on condensate fraction as shown in Fig. 6. The bose condensation temperature is unaffected by the interaction in the Bogoliubov method.

3. Conclusions

In this paper, we investigated the effects of NNN hopping of non-interacting and interacting bosons in cubic lattices on bose condensation temperature and ground state occupancy. We find that the bose condensation temperature is enhanced with increasing t' for bosons in a simple cubic (sc) lattice and decreases for bosons in body-centered cubic (bcc) and face-centered cubic (fcc) lattices. We also find that interaction induced depletion of the condensate is reduced for bosons in a sc lattice while it is enhanced for bosons in bcc and fcc lattices. These results would be relevant to bosons in condensed matter systems in which NNN boson hopping is not negligible. The results could also be applicable to bosons in optical lattices. For instance, it was recently shown that hard-core lattice bosons moving in an optical lattice and interacting with phonon modes of polar molecules trapped in the lattice develops significant NNN hopping amplitudes [21]. There is a hope that several models of strongly correlated quantum many particle systems can be simulated in a controlled manner in optical lattice systems [3,4]. As mentioned earlier, there is also a renewed effort in investigations of bose condensation in crystalline lattices. Further, one of the routes to superconductivity is through the condensation of charged bosons (bipolarons, for example). Furthermore, higher temperature superconductivity may be possible in correlated electron systems by the condensation of charged bosons generated within the electrons system through strong correlation effects [22,23]. Though we are unable to find a concrete example at this juncture, it is not inconceivable that the energy spectra of some of the possible emergent boson modes in strongly correlated lattice electrons systems disperses away in momentum space with significant contributions from NNN hopping amplitudes. Then, our results may have some relevance to these bosons as well.

4. Acknowledgment

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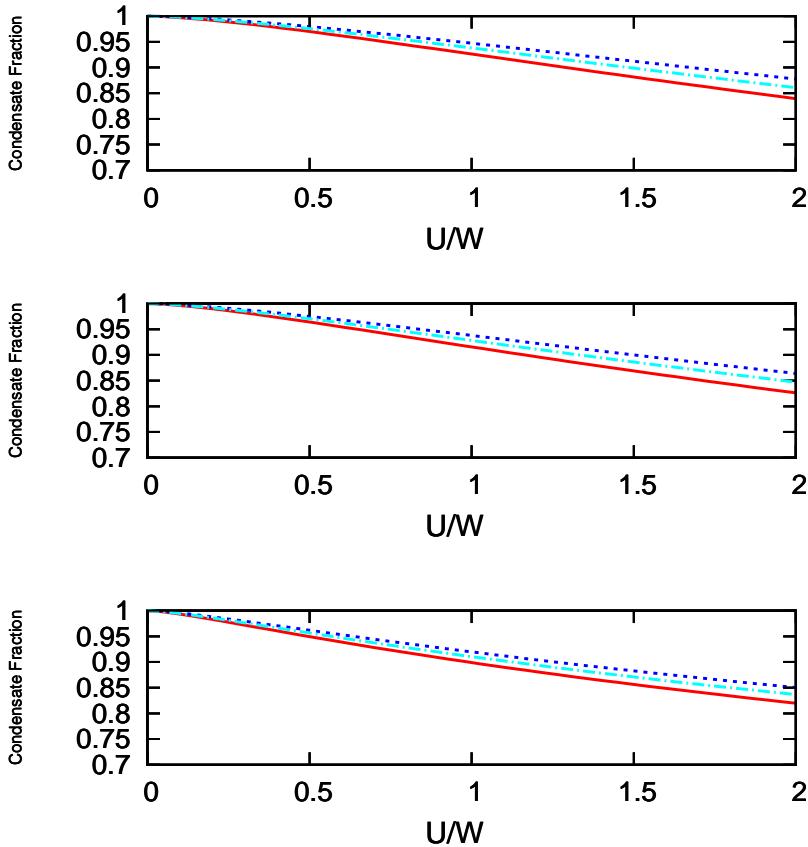


Figure 4. The variation of Condensate fraction (for $T=0$) with U/W of weakly interacting bosons in a sc lattice with NNN hopping t' : $t' = 0$ (solid line), $t' = t/20$ (dash-dot line), $t' = t/10$ (dotted). Here $n = 0.25$ (top panel), $n = 0.4$ (middle panel), $n = 1.5$ (bottom panel).

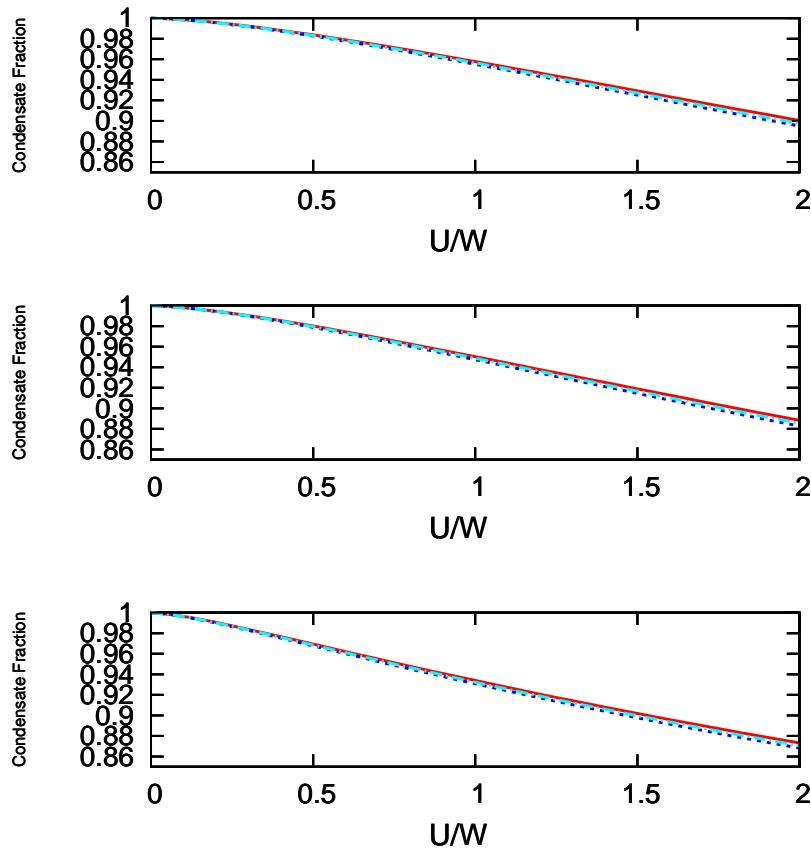


Figure 5. The variation of Condensate fraction (for $T=0$ and $n=0.4$) with U/W of weakly interacting bosons in a bcc lattice with NNN hopping t' : $t'=0$ (solid line), $t'=t/20$ (dash-dot line), $t'=t/10$ (dotted line). Here $n=0.25$ (top panel), $n=0.4$ (middle panel), $n=1.5$ (bottom panel).

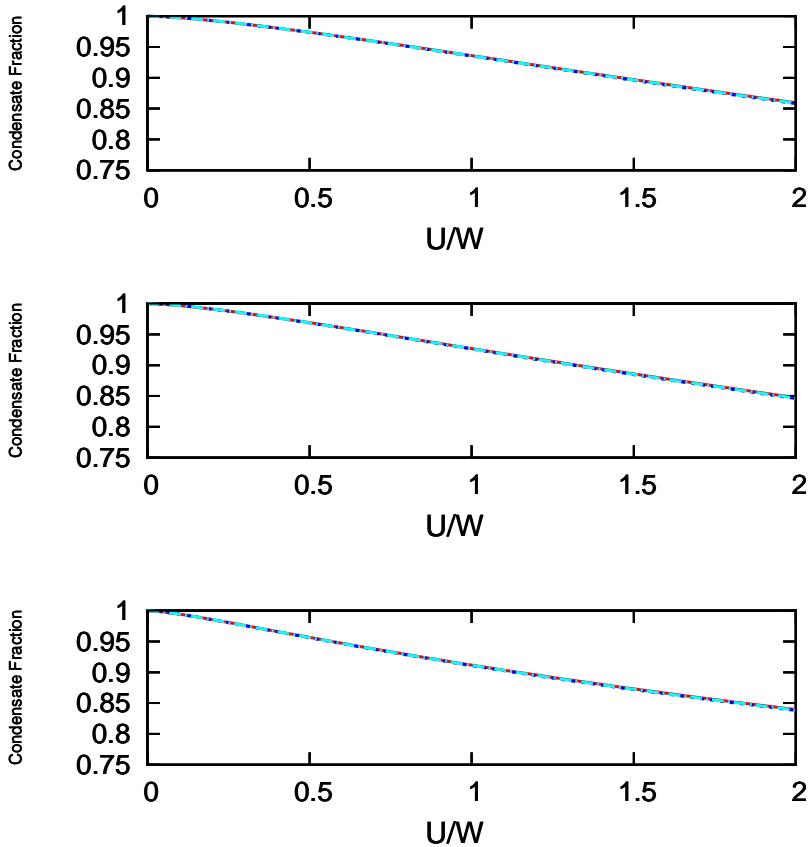


Figure 6. The variation of condensate fraction (for $T=0$ and $n=0.4$) with U/W of weakly interacting bosons in a fcc lattice with NNN hopping t' : $t'=0$ (solid line), $t'=t/20$ (dash-dot line), $t'=t/10$ (dotted line). Here $n=0.25$ (top panel), $n=0.4$ (middle panel), $n=1.5$ (bottom panel).

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